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MACHINE LEARNING INTERATOMIC POTENTIAL FOR AL

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The classic interaction potentials are often used in modern computational methods. Usually the accuracy of these potentials is not enough for different applications. DFT methods can replace classic potentials but they are much more computationally expensive. Machine learning algorithms are known to possess both high accuracy and high operating speed. The aim of our study was to build machine learning potential that can with high accuracy predict the forces acting on each of the atoms in the compound (e.g. during molecular dynamics run).

As a descriptor of the crystal structure that does not depend on translations and rotations we used the idea presented in [1]. The key point there is that the forces are projected on the basis of internal vectors, which are uniquely constructed based on the unit cell. As a result each atom is described by the matrix and the force, acting on it by vector. As a machine learning algorithm, we used a linear regression due to its simplicity and speed. The resultant vector of the parameters in a sense works as interatomic potential. Machine learning potential was implemented in LAMMPS code.

We studied aluminium system. The forces acting on the atoms in the crystalline configurations were predicted within the error 0.04 eV/atom, in the liquid – 0.08 eV/atom. We compared RMSE given by our method and other EAM potentials (Fig. 1). Being trained on Al with a specific density and at specific temperature, the resulting potential is able to predict forces for structures with different densities and temperatures. Using the machine learning potential phonon density of states, entropy and the melting point of Al were calculated. The calculated values are in good agreement with the experimental data.

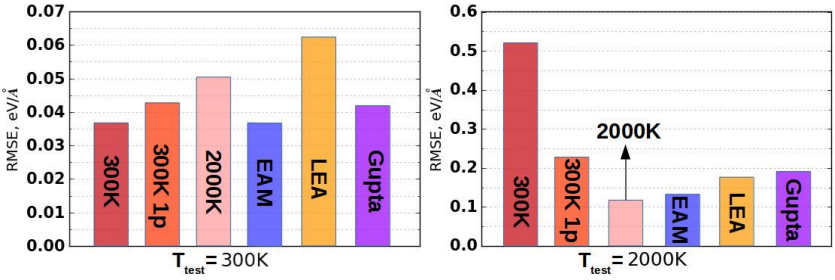

Fig. 1. Comparison of different potentials for Al at 300K (left) and 2000K (right).

1. Li et al., *Phys. Rev. Lett.*, **114**, 2015.